# Lagrangian Investigation of Auto-ignition in a Hydrogen Jet Flame in a Vitiated Co-flow: Animations of Particle Trajectories in Composition Space from PDF Model Calculations

Haifeng Wang and Stephen B. Pope

Sibley School of Mechanical and Aerospace Engineering,

Cornell University, Ithaca, NY 14853, USA

February 5, 2008

**Abstract**

PDF model calculations have been performed of the Cabra lifted hydrogen flame in a vitiated co-flow. Particle trajectories are extracted from the Lagrangian particle method used to solve the modeled PDF equation. The particle trajectories in the mixture fraction-temperature plane reveal (at successive downstream locations): essentially inert mixing between the cold fuel jet and the hot co-flow; the auto-ignition of very lean particles; and, subsequent mixing and reaction, leading to near-equilibrium compositions. The purpose of this paper is to present animations of the particle trajectories obtained using different turbulent mixing models.

## 1 Introduction

We recently reported [1] a PDF modeling study of the $H_2/N_2$ lifted jet flame in a vitiated co-flow, which was studied experimentally by Cabra *et al.*[2]. Particle trajectories are extracted from the Lagrangian particle method used to solve the modeled PDF equation. The particle trajectories in the mixture fraction-temperature ($\xi$-$T$) plane reveal the dominant processes occurring at different locations within the flame. The purpose of this paper is to present some animations of the particle trajectories obtained from these PDF calculations.

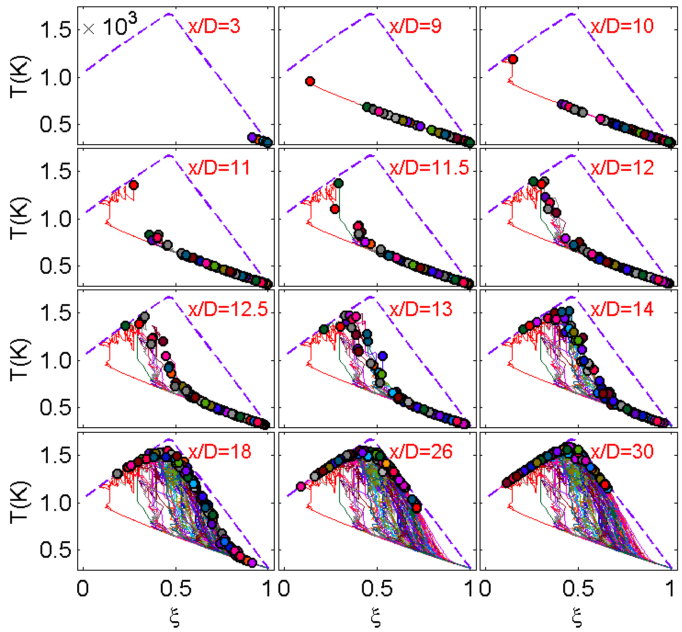


Figure 1: Particle trajectories from the fuel region in the Cabra lifted flame using the EMST model

Full details of the PDF model and its numerical implementation are given in [1]. Calculations are performed using each of the three commonly-used turbulent mixing models. These are: the interaction by exchange with the mean (IEM) model [3] (or, equivalently, the least-mean-square estimation (LMSE) model [4]); the Euclidean minimum spanning tree (EMST) model [5]; and, the modified Curl (MC) model [6, 7].

## 2 Results

Figure 1 shows particle trajectories in the $\xi$-$T$ plane at different axial locations, $x/D$. In each plot: pure fuel corresponds to the lower right corner, $(\xi, T) \approx (1, 300K)$; the co-flow stream corresponds to the middle left, $(\xi, T) \approx (0, 1033K)$; and the dashed line corresponds to chemical equilibrium. The trajectories shown are for particles originating in the fuel stream.

Initially, $(x/D \leq 9)$ the particles move in the plane exclusively by mixing. A particle trajectory due to pure mixing is a nearly straight line between the cold fuel temperature and the hot co-flow temperature. Pure mixing

yields a partially premixed mixture of fuel and oxidizer at different mixture fractions. At about $x/D = 10$, some particles near the oxidizer side start to ignite first: the ignition delay time is shortest for these very lean particles ($\xi \approx 0.05$).

After the rapid auto-ignition of the first few particles, these relatively hot burnt particles (at $x/D > 11$ in Fig. 1) mix with adjacent particles in composition space, thus raising their temperature (and radical concentration) and hence promoting their auto-ignition. Therefore the ignition progressively moves to richer mixtures. This burning process is not exclusively the auto-ignition of the particles. Both reaction and mixing play important roles. Eventually ($x/D \geq 26$) all particles come close to chemical equilibrium. Further discussion on the processes involved is given in [1].

Figures 2 and 3 and show the corresponding trajectories given by the IEM and MC mixing models.

Video 1 and video 2 are animations, showing the evolution of the particles in the $\xi$-$T$ plane as they move downstream, according to the EMST and IEM models, respectively. In the animations, all of the tracked particles are shown (about 1,200), whereas the figures show just 100 trajectories selected randomly.

## Acknowledgements

This work is supported by the Air Force Office of Scientific Research, Grant FA9550-06-1-0048 and by Department of Energy, Grant DE-FG02-90ER. This research was conducted using the resources of the Cornell Theory Center, which receives funding from Cornell University, New York State, federal agencies, foundations, and corporate partners.

## References

[1] Wang, H., Pope, S.B., 2007, Lagrangian investigation of local extinction, re-ignition and auto-ignition in turbulent flames. *Combustion Theory and Modelling,* (submitted).

[2] Cabra, R., Myhrvold, T., Chen, J.-Y., Dibble, R.W., Karpetis, A.N., Barlow, R.W., 2002, Simultaneous laser Raman-Rayleigh-Lif measurements and numerical modeling results of a lifted turbulent H-2/N-2 jet flame in a vitiated coflow. *Proceedings of the Combustion Institute,* **29**, 1881–1888.

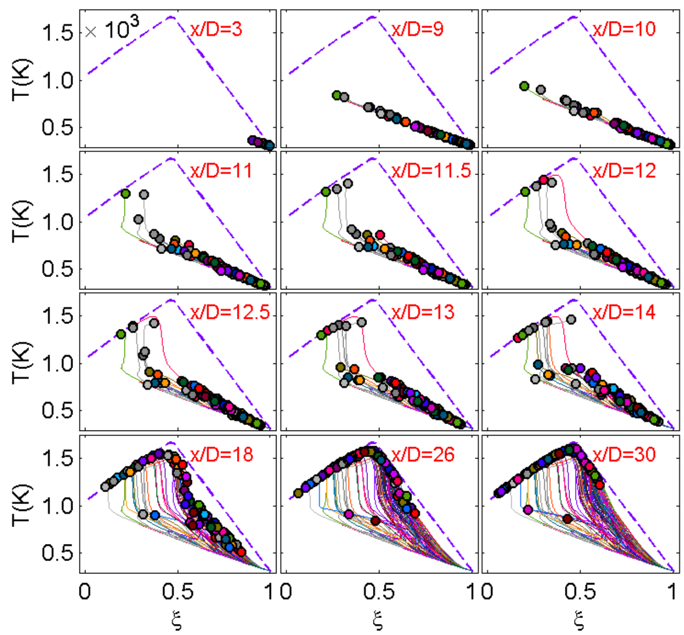


Figure 2: Particle trajectories from the fuel region in the Cabra lifted flame using the IEM model


[3] Villermaux, J., Devillon, J.C., 1972, Reprsentation de la coalescence et de la redispersion des domaines de sgrgation dans un fluide per modle dinteraction phnomnologique. In: *Proceedings of the Second International Symposia on Chemical Reaction,* Elsevier, New York.

[4] Dopazo, C., O'Brien, E.E., 1974, An approach to the autoignition of a turbulent mixture. *Acta Astronautica,* **1**, 1239–1266.

[5] Subramaniam, S., Pope, S.B., 1998, A mixing model for turbulent reactive flows based on Euclidean minimum spanning trees. *Combustion and Flame,* **115**, 487–514.

[6] Janicka, J., Kolbe, W., Kollmann, W., 1979, Closure of the transport-equation for the probability density function of turbulent scalar fields. *Journal of Non-Equilibrium Thermodynamics,* **4**, 47–66.

[7] Nooren, P.A., Wouters, H.A., Peeters, T.W.J., Roekaerts, D., Maas, U., Schmidt, D., 1997, Monte Carlo PDF modelling of a turbulent natural-gas diffusion flame. *Combustion Theory and Modelling,* **1**, 79–96.

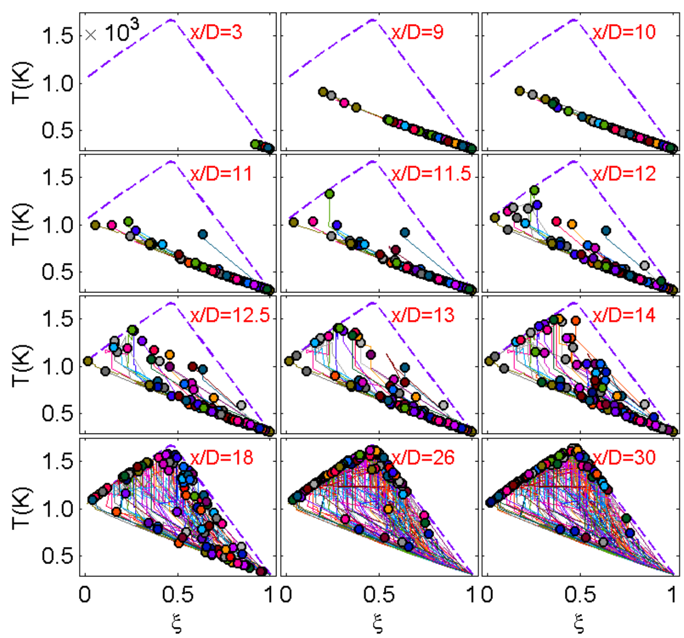


Figure 3: Particle trajectories from the fuel region in the Cabra lifted flame using the MC model